

Physical picture of the gapped excitation spectrum of the one-dimensional Hubbard model

Daniel Braak^{1,2} and Natan Andrei¹

¹ *Department of Physics and Astronomy, Rutgers University, Piscataway, NJ 08855*

² *NEC Research Institute, 4 Independence Way, Princeton, NJ 08540*

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A simple picture for the spectrum of the one-dimensional Hubbard model is presented using a classification of the eigenstates based on an intuitive bound-state Bethe-Ansatz approach. This approach allows us to *prove* a "string hypothesis" for complex momenta and derive an exact formulation of the Bethe-Ansatz equations including all states. Among other things we show that all gapped eigenstates have the Bethe Ansatz form, contrary to assertions in the literature¹. The simplest excitations in the upper Hubbard band are computed: we find an unusual dispersion close to half-filling.

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I. INTRODUCTION

In a recent article² we have introduced a new approach to the derivation of the Bethe Ansatz equations of models with bound states. By bound states we mean that the wave functions contain complex momenta k_j which need to be properly handled in the infinite volume limit. Our approach avoids postulating a "string hypothesis" for the momenta and allows a systematic and simple procedure to derive all eigenstates.

In our approach the Bethe Ansatz is formulated for bound states (and bound states of bound states). These composites are formed on the infinite line and are incorporated systematically as building blocks of the wave functions defined on a finite ring. The composites correspond to *poles* of the respective S-matrices thus guaranteeing their stability under scattering with other particles. This necessitates the introduction of appropriate boundary conditions - Composite Boundary Conditions (CBC) - which respect the construction and allow the formation of *exact strings*. We conjecture that the CBC allow a symmetry - presumably Yangian - to be manifest already at finite volume, a symmetry that is violated by the conventional Periodic Boundary Conditions, hence appearing in the latter case only in the infinite volume limit. We shall refer to this approach as the Bethe Ansatz for Composites (BAC).

The approach is general and applies to any model where complex momenta appear: the Hubbard model, the t-J model, the Anderson model and the multichannel Kondo model among many others. We shall discuss here the Hubbard model in detail and leave the treatment of the other models for later.

The article is organized as follows:

In section II we present the model and construct the class of bound state solutions to the Schrödinger equation of the model and show how to incorporate them as new ansatz functions besides the usual plane waves into the BA. We introduce appropriate boundary conditions (the CBC) to define the model on a finite configuration space, and deduce the BAC equations. A particular class of solutions of the BAC equations is found to underlie the η -pairing and the charge $SU(2)$ symmetry group. Next, we clarify the connection with Takahashi's string hypothesis³, which, we argue, leads to inconsistencies when finite volume corrections are taken into account.

In section III we study the bound state excitation spectrum both in the repulsive and attractive models. In the repulsive case, holding the number of electrons fixed, we find a three parameter excitation, consisting of two gapless *holons* (spinless, carrying charge $-e$) and a bound state residing in the upper Hubbard band (spinless, carrying charge $2e$). The latter is in fact an anti-bound state, corresponding to the formation of a bound pair of electrons with positive binding energy dressed by its interaction with the sea electrons. In the attractive case a dual picture emerges: it corresponds to breaking one of the pairs forming the ground state. The resulting excitation consists of two gapless (renormalized) electrons each carrying charge e and spin $1/2$ and a gapped spinless excitation with charge $-2e$. The gapped excitation is an independent mode only away from half-filling and we give numerical results for its dispersion.

In section IV we summarize our results. Appendix A contains a detailed demonstration of the stability of the two-particle bound state in the presence of other particles with composite boundary conditions.

II. DERIVATION OF THE BAC EQUATIONS

The one-dimensional Hubbard hamiltonian is given by

$$H = \sum_{i=-\infty}^{\infty} -t(\psi_{\sigma,i+1}^{\dagger} \psi_{\sigma,i} + h.c.) + U n_{\uparrow,i} n_{\downarrow,i}. \quad (1)$$

The hamiltonian was diagonalized by Lieb and Wu⁴ in the sector with N particles on a finite ring of length L , with periodic boundary conditions (PBC) imposed on the wavefunction of the N electrons,

$$F(x_1, \dots, x_i, \dots, x_N) = F(x_1, \dots, x_i + L, \dots, x_N) \quad \forall i. \quad (2)$$

The resulting eigenfunction is parameterized, for total spin $S = \frac{1}{2}(N - 2M)$, by N momenta k_j and M spin rapidities λ_γ , satisfying the BA equations^{4,5},

$$e^{ik_j L} = \prod_{\delta=1}^M \frac{\lambda_\delta - \sin k_j - i\frac{u}{4}}{\lambda_\delta - \sin k_j + i\frac{u}{4}} \quad (3)$$

$$\prod_{\delta \neq \gamma}^M \frac{\lambda_\gamma - \lambda_\delta - i\frac{u}{2}}{\lambda_\gamma - \lambda_\delta + i\frac{u}{2}} = \prod_{j=1}^N \frac{\lambda_\gamma - \sin k_j - i\frac{u}{4}}{\lambda_\gamma - \sin k_j + i\frac{u}{4}} \quad (4)$$

where $u = U/t$.

The energy and momentum of the state are then given by

$$E = -2t \sum_j \cos k_j \quad P = \sum_j k_j.$$

The eigenstates of the hamiltonian correspond to the various solutions of eqns (3,4). Real as well as complex solutions need to be considered to obtain a complete spectrum of states.

We shall argue, however, that complex spin rapidities $\{\lambda_\gamma\}$ and complex charge momenta $\{k_j\}$ have a different character although both of them were treated in much the same way in the literature. The former type is associated with the spin degrees of freedom and describes kink/anti-kink bound states. As such they are a many-body phenomenon and make their appearance through complex conjugate solutions of the BA equations for spin rapidities. The existence of these solutions is postulated in the *λ string-hypothesis* about the form of the BA solutions for large number of particles N . Although very plausible, this hypothesis remains unproven up to now⁶.

The latter type - on which we concentrate in this article - is associated with the charge degrees of freedom. In analogy to the spin sector, they were assumed to correspond to complex conjugate solutions of the Lieb - Wu equations for charge rapidities. We will show that they have to be treated differently because they are *not* due to a many-body effect but can be identified with the *elementary* bound states of the hamiltonian, present already in the few-particle sector. They have to be incorporated into the Bethe ansatz ab initio and lead to a set of BA equations, which we call the Bethe ansatz for composites (BAC).

The charge complex momenta were also conjectured to form strings, the so called *$k - \Lambda$ strings*, and Bethe-Ansatz equations were derived based on this hypothesis³. In the thermodynamic limit the BAC equations turn out to be equivalent with those derived using the string-hypothesis for the charge rapidities. This finding does not constitute, however, a proof of the string-hypothesis for a finite system. On the contrary, we shall argue in section II D. that the string-hypothesis for charge bound states leads to an *over-constrained* set of equations, which has in general no solutions for sufficiently large but finite system size L .

We begin by discussing the two string hypotheses separately. To introduce " λ - strings" one assumes complex-conjugate pairs of rapidities $\lambda^\pm = \lambda_0 \pm i\chi$, and introducing them into eq (4) one concludes,

$$\chi = \frac{u}{4} + \mathcal{O}(e^{-\kappa N}) \quad (5)$$

with $\kappa > 0$. More generally, m spin rapidities λ_j are grouped together to form a λ -string of length m :

$$\lambda_j = \lambda_0 + i(m + 1 - 2j)\frac{u}{4} \quad j = 1 \dots m. \quad (6)$$

The solutions with complex λ to the BA equations are driven to the string position (6) in the limit $N \rightarrow \infty$, corresponding to a many particle effect.

The standard classification emerges in terms of *spinons* - chargeless spin-1/2 - objects. The ground state is a singlet, $S = 0$, described by a solution with $M = N/2$ real λ rapidities. The simplest spin excitation corresponds to $M = N/2 - 1$ rapidities, hence $S = 1$. It is found to be a two parameter state and can be interpreted naturally as a symmetric combination of *two* elementary excitations, each carrying spin 1/2, the *spinon* states. To confirm this picture one needs to show that there is also a state with the spinons combined antisymmetrically to form an excited singlet. This can be done by introducing a λ -string of length 2 so that again $M = N/2$ corresponding to a singlet, $S = 0$. This structure of excitations is universal to $SU(2)$ invariant models. It was first observed in the Gross-Neveu model⁷, and subsequently rediscovered in several other models: in the Kondo model⁹, the Heisenberg model¹⁰, the Hubbard model¹¹ or the t-J model¹². Also the spinon - spinon S-matrix, when expressed in terms of rapidities, is identical in these models, and was originally calculated from the Bethe Ansatz in [8]. The fact that quantities such as the quantum numbers of the spinons and their scattering phase shifts are the same in the different models is due to the circumstance that in all of them the interaction has the form of a spin exchange. Thus the spin sector of the various models obeys the same BA equations up to shifts specific to each. As phase shifts and quantum numbers are deduced from simple counting arguments that are independent of those shifts they are identical in spite of a wide variation in dynamics, see [5] for a detailed discussion.

In addition to these spin strings the standard approach assumes “ $k - \Lambda$ strings”, which should describe the charge bound states³. In the simplest case one assumes two complex momenta k^\pm are grouped together with a certain spin rapidity Λ from the set of the λ_γ :

$$\sin k^\pm = \Lambda \mp i \frac{u}{4} + \mathcal{O}(e^{-\frac{|u|}{4}L}), \quad (7)$$

which one proceeds to insert into the Lieb - Wu equations. This procedure is assumed to hold for $k - \Lambda$ strings of any length.

We shall argue in what follows that this approach is flawed (a brief account was given in [2]) and will introduce in its place the BAC approach, which does not rely on a string-hypothesis. We shall argue later that solutions of type (7) *do not* exist for finite L . This is due to the fact that the elementary bound states of (1), to be constructed below, cannot be defined with periodic boundary conditions in the presence of unbound electrons. Therefore, such states - expected to exist in the infinite volume limit - cannot be obtained from finite volume considerations. To obtain a consistent solution at finite volume we need to treat the bound states on an equal footing with the plane wave (scattering) states in the Bethe ansatz, rather than trying to recover them as special solutions, “ $k - \Lambda$ strings”, of the Lieb-Wu equations, which were derived from a Bethe ansatz based on plane waves.

It is amusing to note that already the expression (7) hints that it should not be treated, as is conventionally done, on par with the spin strings. In contrast to the latter the $k - \Lambda$ strings are driven to their asymptotic form in the limit $L \rightarrow \infty$, i.e. in the infinite volume limit without the need for N to be large as well. This suggests that they are not due to a many-body correlation effect as the spin strings (6) and should therefore exist already in the two-particle sector of the Hilbert space.

We proceed now to explain our approach in detail.

A. Elementary bound states and their boundary conditions

The Schroedinger equation of the Hubbard model for N particles reads,

$$\begin{aligned} \sum_i^N F_{a_1 \dots a_N}(n_1, \dots, n_i - 1, \dots, n_N) + F_{a_1 \dots a_N}(n_1, \dots, n_i + 1, \dots, n_N) \\ + U \sum_{i < j}^N \delta_{n_i n_j} F_{a_1 \dots a_N}(n_1, \dots, n_N) = E F_{a_1 \dots a_N}(n_1, \dots, n_N). \end{aligned} \quad (8)$$

The solution of (8) in the two particle sector consists of:

- (i) combination of plane waves $F_{a_1 a_2}(n_1, n_2) = A_{a_1 a_2} e^{i(k_1 n_1 + k_2 n_2)}$ describing unbound particles. These states exist on the infinite line as well as on a finite ring of length L ,
- (ii) bound state solutions which take the following form on the infinite line:

$$F^b(n_1, n_2) = A_{a_1 a_2}^s e^{iq(n_1+n_2)} e^{-\xi(q)|n_1-n_2|}. \quad (9)$$

Here $A_{a_1 a_2}^s$ denotes a spin singlet, i.e. $A_{a_1 a_2}^s = -A_{a_2 a_1}^s$. The parameters q and ξ are related by,

$$\sinh \xi(q) = -\frac{u}{4 \cos q}. \quad (10)$$

The energy of the bound state is $E(q) = -4t \cos q \cosh \xi$ and $\xi \geq 0$. The last condition together with (10) sets a range for q in the interval $[-\pi, \pi]$:

$$\begin{aligned} U > 0 : & \quad |q| \geq \frac{\pi}{2} \\ U < 0 : & \quad |q| \leq \frac{\pi}{2}. \end{aligned} \quad (11)$$

The signs of the energy depends directly on U : it is negative in the attractive case ($U < 0$) and positive in the repulsive case. In the former case the real momentum q (which is half the quantum mechanical (or crystal) momentum: $p = 2q$) lies near the center of the Brillouin zone and in the latter near the edges. Moreover there is a gap in the spectrum $E(q) = U \coth \xi(q)$:

$$\begin{aligned} U > 0 : & \quad E(q) \geq |U| \\ U < 0 : & \quad E(q) \leq -|U|. \end{aligned} \quad (12)$$

The limiting values $\pm|U|$ correspond to $q \rightarrow \pm(\pi/2)$ from above or below according to the sign of U . In both cases $\xi(q)$ tends to infinity at these points. The state with $q = \pi/2$ (equivalent with $q = -\pi/2$) is strictly local - with a zero width wave function both electrons being one on top of the other. The wave function of the local pair is characterized by the crystal momentum $p = \pi$ and energy $E = U$. This local bound state is the only eigenstate of (1), which exists also on a finite ring with even number of lattice sites and plays an important role for the $SU(2)_{charge}$ symmetry, see below.

The bound-state solution (9) corresponds, as it should, to a pole of the appropriate S-matrix (or a zero in its inverse). We proceed to make it manifest.

The scattering matrix between two unbound electrons,

$$S_{ij}(k_i, k_j) = \frac{\sin k_i - \sin k_j + i\frac{u}{2}P_{ij}}{\sin k_i - \sin k_j + i\frac{u}{2}}, \quad (13)$$

is used to construct the conventional scattering solution,

$$F(n_1, n_2) = \mathcal{A} e^{i(k_1 n_1 + k_2 n_2)} (A_{a_1 a_2} \Theta(n_2 - n_1) + [S_{12} A]_{a_1 a_2} \Theta(n_1 - n_2)) \quad (14)$$

where \mathcal{A} denotes the antisymmetrizer and the momenta are real.

To cast expression (9) into this form, rewrite it as,

$$A_{a_1 a_2}^s e^{i(q-i\xi)n_1} e^{i(q+i\xi)n_2} \Theta(n_2 - n_1) + A_{a_1 a_2}^s e^{i(q-i\xi)n_2} e^{i(q+i\xi)n_1} \Theta(n_1 - n_2), \quad (15)$$

which is of the form (14) if we identify: $k_1 = k^- = q - i\xi$ and $k_2 = k^+ = q + i\xi$, provided $[S_{12} A^s]_{a_1 a_2} = 0$. Using now the bound state condition (10), we find, $\sin k^\pm = \sin q \cosh \xi \pm i \cos q \sinh \xi = \sin q \cosh \xi \mp i \frac{u}{4} \equiv \phi(q) \mp i \frac{u}{4}$. We have used the following notation:

$$\phi(q) = \Re(\sin k^\pm) = \sin q \left(1 + \frac{u^2}{16 \cos^2 q} \right)^{1/2}. \quad (16)$$

Thus, inserting these values into eq.(13) we have,

$$S_{12}(k^-, k^+) = \frac{1}{2}(\mathbf{1} + P_{12}). \quad (17)$$

Observe that S_{12} vanishes indeed for the singlet ($P_{12} = -1$): $[S_{12} A^s]_{a_1 a_2} = 0$, while, $S_{21} = S_{12}^{-1} = S_{12}(k^+, k^-)$, is in turn undefined¹³: the complex momentum satisfying the bound state condition (10) is placed on the *pole* - a standard result of scattering theory.

Hence (14) gives correctly the wavefunction (9) after antisymmetrization as the amplitude $e^{\xi x}$ which diverges in interval $x > 0$ is projected out:

$$F(n_1, n_2) = \mathcal{A} e^{i(q-i\xi)n_1} e^{i(q+i\xi)n_2} A_{a_1 a_2}^s \Theta(n_2 - n_1) = A_{a_1 a_2}^s e^{iq(n_1+n_2)} e^{-\xi|n_1-n_2|}. \quad (18)$$

We conclude that the bound state can be written in the usual Bethe ansatz form (14) if we allow for singular S-matrices like (17).

If we seek an analogue of this bound state solution in the framework of PBC we find that the momentum is not placed at the pole of the S-matrix. Assume two electrons on the ring with L sites. Let us consider a singlet wave function in the two-particle sector, $N = 2$, and $S = 0$, (i.e. $M = 1$). The equations (3,4) read,

$$e^{ik_j L} = \frac{\lambda - \sin k_j - i\frac{u}{4}}{\lambda - \sin k_j + i\frac{u}{4}}, \quad j = 1, 2 \quad (19)$$

$$1 = \prod_{j=1}^2 \frac{\lambda - \sin k_j - i\frac{u}{4}}{\lambda - \sin k_j + i\frac{u}{4}}. \quad (20)$$

Now we look for solutions of (19,20) with complex k_j , of the form $k_{1,2} = q \pm i\xi$. Inserting into the equations we find that the spinon parameter λ is given by $\lambda = \phi(q)$ and ξ satisfies the following equation

$$e^{-2\xi L} = \left(\frac{\cos q \sinh \xi + \frac{u}{4}}{\cos q \sinh \xi - \frac{u}{4}} \right)^2, \quad (21)$$

which means,

$$|\cos q| \sinh \xi - \frac{|u|}{4} \sim e^{-\xi L} \quad (22)$$

for finite L . It follows that the bound state momentum in a finite system with PBC according to the Lieb-Wu equations deviates from the pole in the corresponding S-matrix by a term of order $e^{-\xi L}$. This makes S_{12} regular and leads to a $F(n_1, n_2)$ periodic in each variable separately, because in each sector of configuration space there is also an amplitude with the exponentially diverging solution. These amplitudes are forbidden only for $L \rightarrow \infty$. The fact, that the bound state parameter *does not* satisfy the pole condition (10) for finite L renders the bound state unstable when scattered on additional particles¹⁴. To avoid this problem, we have to introduce boundary conditions, which allow the state (9) to exist in a finite system. This is done in the next section.

B. The Composite Boundary Conditions (CBC) and the Bethe Ansatz for Composites (BAC)

We proceed to introduce boundary conditions which allow us to incorporate bound-states consistently, bypassing the unsatisfactory “string hypothesis”. We shall show that the Composite Boundary Conditions (i) define a complete Hilbert space spanned by 4^L states for finite volume L , (ii) lead in the infinite volume limit to the conventional quantization of the infinite line, (iii) respect the formation of the bound states. We conjecture that they allow, already for finite volume, a symmetry expected to hold only in the infinite volume limit. The presence of this symmetry may underlie the *exact* form of our Bethe Ansatz equations.

To impose a boundary condition on particle j we have to find a path in configuration space leading from region $x_j < x_1 < x_2 \dots < x_N$ to region $x_1 < x_2 \dots < x_N < x_j$. If j belongs to a bound state, the corresponding product of S-matrices is necessarily singular. We can avoid the singularity by taking the two members j^- and j^+ simultaneously around the ring of circumference L , by imposing the following modified boundary condition for bound states,

$$F(x_1 \dots, x_{j^-}, \dots, x_{j^+}, \dots, x_N) = F(x_1 \dots, x_{j^-} + L, \dots, x_{j^+} + L, \dots, x_N) \quad (23)$$

corresponding to periodicity of the center of mass coordinate. For unbound particles we retain conventional periodicity. Two new nonsingular S-matrices arise. The S-matrix of a bound pair with an unbound particle, $S_{i(j^-j^+)}^{ub}$, and the S-matrix, $S_{(i^-i^+)(j^-j^+)}^{bb}$, between two bound pairs. These are in addition to the usual S_{ij}^{uu} given by (13) valid for both k_i and k_j real.

The factorization property of the S-matrices (13) makes the following construction possible: Because of the validity of the Yang Baxter relation it is sufficient to consider only amplitudes in which the two members of the bound pair, with momenta $k^\pm = q \pm i\xi$, are neighbors. Obviously the scattering matrix of the pair off an unbound particle with momentum k is,

$$S_{1(23)}^{ub} = S_{13}^{uu}(k, k^+) S_{12}^{uu}(k, k^-), \quad (24)$$

and we find (see appendix A),

$$S_{1(23)}^{ub}(k, q) = \frac{\sin k - \phi(q) - i\frac{u}{4}}{\sin k - \phi(q) + i\frac{u}{4}}. \quad (25)$$

S^{ub} is a scalar in spin-space, and acts as a pure (momentum dependent) phase shift on the wavefunctions. The bound state is *stable*, its internal wavefunction is not affected by the scattering with the unbound particle. In other words, it couples directly only to the charge degrees of freedom via the phase-shift (25). In an analogous way we derive $S_{(12)(34)}^{bb}(q_a, q_b)$ by using,

$$S_{(12)(34)}^{bb} = S_{1(34)}^{ub}(k_a^-, q_b) S_{2(34)}^{ub}(k_a^+, q_b) \quad (26)$$

with the result

$$S_{(12)(34)}^{bb}(q_a, q_b) = \frac{\phi(q_a) - \phi(q_b) - i\frac{u}{2}}{\phi(q_a) - \phi(q_b) + i\frac{u}{2}}. \quad (27)$$

We proceed now to derive the Bethe-Ansatz equations. As S^{ub} and S^{bb} commute with each other and all the S^{uu} 's they do not enter the self consistency BA equations (4). This fact is responsible for the (partial) decoupling of the bound states from the free particles which are correlated via the spinon parameters λ_γ . Assume $N = N^u + 2N^b$ electrons, where $2N^b$ particles are in bound states characterized by momenta q_l , $l = 1 \dots N^b$ and N^u particles are in plane wave states given by momenta k_j , $j = 1 \dots N^u$. The total spin S is given by $S = \frac{1}{2}(N^u - 2M)$, where M denotes the number of spin-lowering operators in the algebraic Bethe ansatz.

One proceeds to construct the Z -matrix which takes a particle or a bound pair around the ring L . For a particle j in an unbound state it takes the form,

$$Z_j = S_{1j}^{uu} \dots S_{N^u j}^{uu} S_{1j}^{ub} \dots S_{N^b j}^{ub} \quad (28)$$

with eigenvalue $z_j = e^{ik_j L}$. The last N^b S-matrices are phases. Diagonalizing Z_j is a standard procedure and we find the BA equations,

$$e^{ik_j L} = \prod_{\delta=1}^M \frac{\lambda_\delta - \sin k_j - i\frac{u}{4}}{\lambda_\delta - \sin k_j + i\frac{u}{4}} \prod_{l=1}^{N^b} \frac{\phi(q_l) - \sin k_j - i\frac{u}{4}}{\phi(q_l) - \sin k_j + i\frac{u}{4}} \quad (29)$$

$$\prod_{\delta \neq \gamma}^M \frac{\lambda_\gamma - \lambda_\delta - i\frac{u}{2}}{\lambda_\gamma - \lambda_\delta + i\frac{u}{2}} = \prod_{j=1}^{N^u} \frac{\lambda_\gamma - \sin k_j - i\frac{u}{4}}{\lambda_\gamma - \sin k_j + i\frac{u}{4}} \quad (30)$$

Similarly the Z -matrix for a bound pair determines its momentum, q_l , and is given by,

$$Z_{(ij)} = S_{1(ij)}^{ub} \dots S_{N^u(ij)}^{ub} S_{(r_1^-, r_1^+)(ij)}^{bb} \dots S_{(r_{N^b}^-, r_{N^b}^+)(ij)}^{bb} \quad (31)$$

with eigenvalue $z_{(ij)} = e^{2iq_l L}$. The resulting BA equations read,

$$e^{2iq_l L} = \prod_{j=1}^{N^u} \frac{\sin k_j - \phi(q_l) - i\frac{u}{4}}{\sin k_j - \phi(q_l) + i\frac{u}{4}} \prod_{n \neq l}^{N^b} \frac{\phi(q_n) - \phi(q_l) - i\frac{u}{2}}{\phi(q_n) - \phi(q_l) + i\frac{u}{2}} \quad (32)$$

The equations (29,30,32) replace the set (3,4) in the presence of two-particle bound states. These bound states, however, are not the only multi-particle complexes which are allowed by the hamiltonian. We can infer the existence of higher composites by looking for zeros and poles of the S-matrix for two two-particle bound states (27). The zero of the bound - state S-matrix, (27), is at, $\phi(q_a) - \phi(q_b) = i\frac{u}{2}$, corresponding to complex q 's. Choosing $\phi_{1,2}^2 = \phi_0^2 \pm i\frac{u}{4}$, we find the four momenta of this “double” bound state, the so-called quartet⁵,

$$\begin{aligned}
\sin k_1^2 &= \phi_1^2 + i\frac{u}{4} \\
\sin k_2^2 &= \phi_1^2 - i\frac{u}{4} \\
\sin k_3^2 &= \phi_2^2 + i\frac{u}{4} \\
\sin k_4^2 &= \phi_2^2 - i\frac{u}{4}.
\end{aligned} \tag{33}$$

In other words,

$$\begin{aligned}
k_1^2 &= \pi - \arcsin(\phi_0^2 + i\frac{u}{2}) \\
k_2^2 &= \arcsin(\phi_0^2) \\
k_3^2 &= \pi - \arcsin(\phi_0^2) \\
k_4^2 &= \pi - \arcsin(\phi_0^2 - i\frac{u}{2}).
\end{aligned} \tag{34}$$

Again we can derive the S-matrix of this state with the unbound and the simple bound state. The latter follows from the former upon application of a relation similar to (26). We find

$$S_{k\phi_0^2}^{u(bb)} = \frac{\sin k - \phi_0^2 - i\frac{u}{2}}{\sin k - \phi_0^2 + i\frac{u}{2}} \tag{35}$$

In general there are bound complexes of $2m$ electrons, (m -complexes), corresponding to a pole in the S-matrix of a $(m-1)$ -complex with a simple bound pair, (a 1-complex). They are parameterized by m complex numbers $\{\phi_j^m, j = 1 \dots m\}$ in the complex plane:

$$\phi_j^m = \phi_0^m + (m+1-2j)i\frac{u}{4} \tag{36}$$

corresponding to $2m$ complex momenta,

$$\begin{aligned}
k_1^m &= \pi - \arcsin(\phi_0^m + im\frac{u}{4}) \\
k_2^m &= \arcsin(\phi_0^m + i(m-2)\frac{u}{4}) \\
k_3^m &= \pi - \arcsin(\phi_0^m + i(m-2)\frac{u}{4}) \\
&\vdots \\
k_{2m-1}^m &= \pi - \arcsin(\phi_0^m - i(m-2)\frac{u}{4}) \\
k_{2m}^m &= \pi - \arcsin(\phi_0^m - i(m)\frac{u}{4})
\end{aligned} \tag{37}$$

In fact, these correspond to the bound complexes conjectured by Takahashi³.

We proceed along the same lines as before: The S-matrix of an m -complex with an unbound particle is,

$$S_{k\phi_0^m}^{u(m)} = \frac{\sin k - \phi_0^m - im\frac{u}{4}}{\sin k - \phi_0^m + im\frac{u}{4}} \tag{38}$$

allowing us to derive the S-matrix of an m -complex with an n -complex:

$$S_{\phi_0^n, \phi_0^m}^{(m)(n)} = \frac{\phi_0^m - \phi_0^n - |n-m|i\frac{u}{4}}{\phi_0^m - \phi_0^n + |n-m|i\frac{u}{4}} \frac{\phi_0^m - \phi_0^n - (n+m)i\frac{u}{4}}{\phi_0^m - \phi_0^n + (n+m)i\frac{u}{4}} \prod_{l=1}^{\min(m,n)-1} \left(\frac{\phi_0^m - \phi_0^n - (|n-m|+2l)i\frac{u}{4}}{\phi_0^m - \phi_0^n + (|n-m|+2l)i\frac{u}{4}} \right)^2. \tag{39}$$

If we impose the composite boundary condition on the m -complexes,

$$F(x_1 \dots, x_1^{(m)}, \dots, x_{2m}^{(m)}, \dots, x_N) = F(x_1 \dots, x_1^{(m)} + L, \dots, x_{2m}^{(m)} + L, \dots, x_N) \tag{40}$$

where the $\{x_i^{(m)}\}$ are the coordinates of the members of the m -complex, we are led immediately to the corresponding eigenvalue of the m -complex transfer matrix, (recall, all bound states are spin singlets):

$$\exp(iL \sum_l k_l^m) = \exp(iL[-2\Re \arcsin(\phi_0 + mi\frac{u}{4}) + (m+1)\pi]) \equiv e^{iq^m(\phi_0)L}. \quad (41)$$

In this way we get the full BAC equations, a generalization of (29,30,32):

$$e^{ik_j L} = \prod_{\delta=1}^M \frac{\lambda_\delta - \sin k_j - i\frac{u}{4}}{\lambda_\delta - \sin k_j + i\frac{u}{4}} \prod_{\substack{(a,n) \\ \phi_0^{(a,n)}, k_j}} S_{\phi_0^{(a,n)}, k_j}^{(n)u} \quad (42)$$

$$\prod_{\delta \neq \gamma}^M \frac{\lambda_\gamma - \lambda_\delta - i\frac{u}{2}}{\lambda_\gamma - \lambda_\delta + i\frac{u}{2}} = \prod_{j=1}^{N^u} \frac{\lambda_\gamma - \sin k_j - i\frac{u}{4}}{\lambda_\gamma - \sin k_j + i\frac{u}{4}} \quad (43)$$

$$e^{iq^m(\phi_0^{(b,m)})L} = \prod_{(a,n) \neq (b,m)} S_{\phi_0^{(a,n)}, \phi_0^{(b,m)}}^{(n)(m)} \prod_j^{N^u} S_{k_j \phi_0^{(b,m)}}^{u(m)} \quad (44)$$

where the index (a, n) runs over the set of all n -complexes present. These equations were also derived by Takahashi in [3], within the framework the $k - \Lambda$ string hypothesis. His procedure, however, involves discarding finite volume corrections in equations written for finite volume. Our derivation makes no use of this hypothesis as all charge bound states are consistently incorporated *ab initio*.

To discuss the nature of the eigenstates and count them it is convenient to consider (44) in a logarithmic form,

$$q^m(\phi_0^{(b,m)})L = \sum_{(a,n) \neq (b,m)} \Theta_{nm}(\phi_0^{(b,m)} - \phi_0^{(a,n)}) - 2\pi J_m^b \quad (45)$$

where,

$$\begin{aligned} \Theta_{nm}(x) &= \theta\left(\frac{x}{|n-m|}\right) + 2\theta\left(\frac{x}{|n-m|+2}\right) + \dots 2\theta\left(\frac{x}{|n-m|-2}\right) + \theta\left(\frac{x}{n+m}\right) & n \neq m \\ &= 2\theta\left(\frac{x}{2}\right) + 2\theta\left(\frac{x}{4}\right) + \dots 2\theta\left(\frac{x}{2n-2}\right) + \theta\left(\frac{x}{2n}\right) & n = m \end{aligned}$$

with $\theta(x) = -2 \tan^{-1}(x\frac{4}{u})$.

Each allowed choice of quantum numbers $\{J_m^b\}$ uniquely labels the eigenstate, and the allowed ranges can be deduced³ from eqn(45), (a derivation for the case $m = 1$ is given in the next section),

$$|J_m^b| < \frac{1}{2}(L - N^u - \sum_{n>0} t_{nm} M_n). \quad (46)$$

Here M_n denote the number of n -complexes, t_{nm} is defined as $t_{nm} = 2\min(n, m) - \delta_{nm}$. These equations are the starting point for counting the number of states of the model.

We end this subsection by showing that the dimensions of the Hilbert spaces for CBC and PBC are the same. The dimension of the Hilbert space with CBC is larger or equal to the dimension of the space with PBC:

$$\dim \mathcal{H}_{CBC} \geq \dim \mathcal{H}_{PBC} \quad (47)$$

as each vector in \mathcal{H}_{PBC} lies also in \mathcal{H}_{CBC} . On the other hand, there is a one-to-one relation between states in \mathcal{H}_{CBC} , not satisfying PBC and states in \mathcal{H}_{PBC} . If one writes a vector in \mathcal{H}_{CBC} as function of the center-of-mass and relative coordinates

$$F(x_1, \dots, x_N) = F(X_{c.m.}, x_i - x_j)$$

one has the injective mapping $\Phi(F)$ onto \mathcal{H}_{PBC} :

$$\Phi(F) = F(X_{c.m.}, [x_i - x_j] \bmod L) \quad (48)$$

because the value of the wavefunction $F(x_1, \dots, x_N)$ outside the interval $|x_i - x_j| < L/2$ is completely determined by its value inside. It follows

$$\dim \mathcal{H}_{CBC} = \dim \mathcal{H}_{PBC} \quad (49)$$

C. Global Symmetries and the Bethe-Ansatz nature of all Eigenstates

We begin by considering the global symmetries of the model whose eigenvalues (partially) label the eigenstates. We shall show, among other things, that all the eigenstates of the model are of the Bethe Ansatz form. This is in contrast to claims by Eßler, Korepin and Schoutens¹ that only the highest weight states have the Bethe Ansatz form while the rest cannot be represented this way.

First, we have the spin $SU(2)$ -symmetry, with

$$\hat{S}_z = \frac{1}{2} \sum_i n_{\uparrow,i} - n_{\downarrow,i}, \quad \hat{S}^- = \sum_i \psi_{\downarrow,i}^\dagger \psi_{\uparrow,i}, \quad \hat{S}^+ = \sum_i \psi_{\uparrow,i}^\dagger \psi_{\downarrow,i}$$

The spin operators commute with the particle number operator, $\hat{N} = \sum_i n_{\uparrow,i} + n_{\downarrow,i}$, and the application of the spin-lowering operator \hat{S}^- does not lead to a change in particle number.

The spin highest weight state $|S = S_z = (1/2)(N - 2M)\rangle$ is defined by a solution $\{\lambda_\gamma, \gamma = 1 \dots M\}$, all λ_γ finite. To obtain another member of the multiplet consider the solution with $M + 1$ spin rapidities $\{\lambda_1 \dots \lambda_M, \lambda_0\}$ and $\lambda_0 = \infty$. It formally satisfies (42,43), and corresponds to the state obtained from $\{\lambda_1 \dots \lambda_M\}$ by an application of \hat{S}^- , since $B(\lambda) \rightarrow \hat{S}^-/\lambda$, when $\lambda \rightarrow \infty$, in the framework of the algebraic Bethe ansatz. Repeated application of \hat{S}^- will generate the whole $SU(2)_{spin}$ multiplet from $\{\lambda_\gamma\}$, which consists of $2S + 1$ states, i.e. we will find a zero wavefunction for more than $2S$ spin rapidities equal to infinity. A consistent way of defining this process is provided by considering an anisotropic version of the spin sector. New complex roots, denote them as λ^- - roots, are generated with π/γ as their imaginary part, where γ is the anisotropy parameter. When $\gamma \rightarrow 0$ isotropy is regained and the λ^- - roots are sent to infinity in a controllable way, generating the Bethe Ansatz states that complete the multiplet^{19,20}.

An even simpler argument holds in the case of the charge $SU(2)$ symmetry. It is defined on a ring with L sites (L even), as follows^{16,17},

$$\eta_z = \frac{1}{2}(L - \hat{N}), \quad \eta^+ = \sum_j (-1)^j \psi_{j\uparrow}^\dagger \psi_{j\downarrow}^\dagger, \quad \eta^- = \sum_j (-1)^j \psi_{j\downarrow} \psi_{j\uparrow}. \quad (50)$$

The algebra is consistent with the CBC since the η^\pm operators create (destroy) local pairs - see below. The symmetry is manifest when one adds a chemical potential term with $\mu = -U/2$ to the hamiltonian:

$$H_{h.f.} = \sum_{i=-\infty}^{\infty} -t(\psi_{\sigma,i+1}^\dagger \psi_{\sigma,i} + h.c.) + U n_{\uparrow,i} n_{\downarrow,i} - \frac{U}{2} \hat{N} \quad (51)$$

This choice of μ corresponds to a half-filled system in the grand canonical formalism. We have

$$[H_{h.f.}, \eta^\pm] = 0 \quad [\hat{N}, \eta^\pm] = \pm 2\eta^\pm \quad (52)$$

Clearly, the symmetry generators η^\pm mix sectors with different particle number.

In terms of the BAC equations the η -symmetry has a simple explanation: Consider a given eigenstate of H , say $|\psi\rangle = |\psi(\{\lambda_\gamma\}, \{k_j\}, \{q_l\})\rangle$ with N particles characterized by unbound momenta $\{k_j\}$ and bound momenta $\{q_l\}$, as well as spin content given by $\{\lambda_\gamma\}$. Acting with the operator η^+ adds to it a bound pair with $q = \pi/2$ and crystal momentum $p = \pi$:

$$\eta^+ |\psi(\{\lambda_\gamma\}, \{k_j\}, \{q_l\})\rangle = |\psi'(\{\lambda_\gamma\}, \{k_j\}, \{q_l, \pi/2\})\rangle. \quad (53)$$

(We have assumed $q_l \neq \pi/2, \forall l$). Note that for a finite system, namely with CBC for $L < \infty$, the state with $q = \pi/2$ exists for even L . The state $|\psi'\rangle$ is again an eigenstate of H , because the S-matrix between the bound pair with $q = \pi/2$ and all other complexes is the identity (total transmission), - see (38), (39) and recall: $\phi(\pi/2) = \infty$. The state $|\psi'\rangle$ has then $N' = N + 2$ particles and its energy is

$$H|\psi'\rangle = [E(\psi) + U]|\psi'\rangle \quad (54)$$

since adding a bound pair at the edge, $q = \pi/2$, corresponds to $\Delta E = U$, see eqn (12) and subsequent discussion. Thus,

$$H_{h.f.}|\psi'\rangle = E_{h.f.}(\psi)|\psi'\rangle. \quad (55)$$

$|\psi'\rangle$ is degenerate with $|\psi\rangle$ and the symmetry is manifest. We now proceed to add several pairs with $q = \pi/2$ to the state $|\psi\rangle$. These states have zero width - $\xi(\pm\pi/2) = \infty$ - and they behave as hard-core bosons: The S-matrix among themselves is $S = -1$, corresponding to total reflection. The maximal number of applications of η^+ to $|\psi\rangle$ is restricted to $L - N$, the number of available lattice sites. Here N includes bound as well as unbound states - the former with $q \neq \pm\pi/2$ and thus $\xi \neq \infty$, giving them a finite spread. For more than $L - N$ applications of η^+ the state is annihilated due to the Pauli principle. The total number of states degenerate under the η -symmetry is therefore $L - N + 1$. This degeneracy coincides with the dimension of the $SU(2)_{charge}$ multiplet for $S_{charge} = S_{z,charge} = \frac{1}{2}(L - N)$, which is the eigenvalue of η_z applied to $|\psi\rangle$. It follows that the Bethe state $|\psi\rangle$ is a lowest weight state of this symmetry, and all members of the multiplet have the appropriate Bethe Ansatz form²¹.

Actually, our construction goes further. We see from (54), that the η -symmetry can be used to group the eigenstates of H into multiplets even away from half-filling when the $SU(2)_{charge}$ symmetry is explicitly broken: The energies of the $L - N + 1$ states in the multiplet are equally spaced with $E_{i+1} - E_i = U - 2\mu$.

D. Periodic Boundary Conditions (PBC), and Takahashi's conjecture

In this section we shall discuss the approach to the bound states within the usual scheme - imposing periodic boundary conditions.

Defining the system on a finite ring L and imposing PBC (a multi-torus geometry) we have seen above that the parameters q and ξ of a normalizable eigenstate of H in the two-particle sector deviate from the pole (given by eq. (10)) in the scattering matrix by a term of order $e^{-\frac{|u|}{4}L}$:

$$|\cos q| \sinh \xi - \frac{|u|}{4} \sim e^{-\xi L} \sim e^{-\frac{|u|}{4}L} \quad \text{for } |q| \text{ resp. } |q - \pi| \ll \pi/2. \quad (56)$$

This deviation is responsible for the instability of this state when a third particle is added with real momentum k ¹⁴. The S-matrix S^{ub} is no longer a pure phase, and alters the spin structure of the bound state. There is a finite (although exponentially small) probability for the bound state to switch from the spin singlet to the spin triplet state upon passing through the third particle. As the wavefunction has to be antisymmetric in configuration space, we have an *anti-bound state* which cannot satisfy periodic boundary conditions and is clearly forbidden in the infinite volume limit. That means that PBC contradict the local properties of the interaction encoded in the pole structure of the S-matrix, while the CBC are consistent with it. The coordinate space of the system with the CBC is not a multi-torus, but has a more complicated topological structure which, however, turns into the infinite line for $L \rightarrow \infty$ as does the geometry of PBC.

One might still look for the analogues of the normalizable two-particle state (and higher composites) on a finite ring with PBC - solutions to the Lieb-Wu equations (3,4) with complex momenta. It is clear that some of the states must contain complex momenta because otherwise the subspace containing doubly occupied sites would be projected out in the $U \rightarrow \infty$ limit¹¹.

Takahashi's $k - \Lambda$ string hypothesis³ assumes that the states containing complex momenta are of the special form (7) for large L , i.e. they become elementary bound states for infinite volume. Therefore, using the string hypothesis one obtains BA equations similar to those for CBC (42,43,44), but containing correction terms. In fact, if one drops the corrections $\sim e^{-\frac{|u|}{4}L}$ then Takahashi's equations do not describe PBC but instead CBC for finite L . The proof of completeness of the Bethe ansatz solutions given in [18] uses Takahashi's equations for finite L and counts not the number of states on a finite ring for which they are approximate but on the CBC geometry, where these equations become *exact*. But is Takahashi's hypothesis correct for PBC and finite L when the terms proportional to $e^{-\frac{|u|}{4}L}$ do not vanish?

We argue now, by examining the consequences of this assumption, that this is not the case and the complete spectrum for PBC is (in general) not given by $k - \Lambda$ string solutions to (3,4).

We begin by reviewing Takahashi's approach in a simple case with no spin-strings or higher composites present. We assume N^e electrons $2N^b$ of them carrying complex momenta $k_l^\pm = q_l \pm i\xi_l$. In addition we assume $M = N^b + M^u$ real spin rapidities $\{\Lambda_l, \lambda_\gamma; l = 1 \dots N^b; \gamma = 1 \dots M^u\}$, N^b of them, $\{\Lambda_l\}$, associated with the complex momenta as follows,

$$\sin k_l^\pm \equiv \phi(q_l) \mp i\chi_l = \Lambda_l \mp i\frac{u}{4} + \mathcal{O}(e^{-\xi_l L}). \quad (57)$$

Plugging this form into (3,4) one finds,

$$e^{ik_j L} = \prod_{\delta=1}^{M^u} \frac{\lambda_\gamma - \sin k_j - i\frac{u}{4}}{\lambda_\gamma - \sin k_j + i\frac{u}{4}} \prod_{l=1}^{N^b} \frac{\Lambda_l - \sin k_j - i\frac{u}{4}}{\Lambda_l - \sin k_j + i\frac{u}{4}} \quad (58)$$

$$\prod_{\delta \neq \gamma}^{M^u} \frac{\lambda_\gamma - \lambda_\delta - i\frac{u}{2}}{\lambda_\gamma - \lambda_\delta + i\frac{u}{2}} = \prod_{j=1}^{N^u} \frac{\lambda_\gamma - \sin k_j - i\frac{u}{4}}{\lambda_\gamma - \sin k_j + i\frac{u}{4}} (1 + \mathcal{E}_\gamma) \quad (59)$$

$$\prod_{\delta=1}^{M^u} \frac{\Lambda_l - \lambda_\delta - i\frac{u}{2}}{\Lambda_l - \lambda_\delta + i\frac{u}{2}} = \prod_{j=1}^{N^u} \frac{\Lambda_l - \sin k_j - i\frac{u}{4}}{\Lambda_l - \sin k_j + i\frac{u}{4}} (e^{i\psi_l} + \mathcal{E}_l) \quad (60)$$

$$e^{2iq_l L} = \prod_{\gamma=1}^{M^u} \frac{\lambda_\gamma - \Lambda_l - i\frac{u}{2}}{\lambda_\gamma - \Lambda_l + i\frac{u}{2}} \prod_{n \neq l}^{N^b} \frac{\Lambda_n - \Lambda_l - i\frac{u}{2}}{\Lambda_n - \Lambda_l + i\frac{u}{2}} (e^{i\psi_l} + \mathcal{E}_l). \quad (61)$$

Here $\{\mathcal{E}\}$ denote terms of order $e^{-\kappa L}$, with $\kappa \geq |\frac{u}{4}|$. The phase $e^{i\psi_l}$ is defined as

$$e^{i\psi_l} = -\frac{\Lambda_l - \sin k_l^+ - i\frac{u}{4}}{\Lambda_l - \sin k_l^- + i\frac{u}{4}}. \quad (62)$$

Now the set (58 - 61) consists of $N^u + M^u + 2N^b$ coupled algebraic equations for the variables $\{k_j, \lambda_\gamma, q_l, \Lambda_l\}$, i.e. the number of variables coincides with the number of equations²². But in the $L \rightarrow \infty$ limit, Λ_l is not independent from q_l , because of (57): The Λ_l should be eliminated from the set together with the N^b parameters ψ_l , which do not describe physical properties of the state. Takahashi did this by substituting eq. (60) into (61) after dropping the \mathcal{E} -terms. The resulting equations are the set (29,30,32). It is clearly consistent, as it can be derived using BAC. The question arises whether the finite size correction terms in (58 - 61) can spoil the consistency for finite L . We proceed now to show that this is the case in general.

Let us assume there is a consistent solution $\{k_j(L), \lambda_\gamma(L), q_l(L), \Lambda_l(L), \psi_l(L)\}$ of (58 - 61) for arbitrary (large) L . We define the set $\{k_j^0(L), q_l^0(L), \lambda_\gamma^0(L), \Lambda_l^0(L) = \phi(q_l^0(L)), \psi_l^0(L)\}$ as the solution of the zeroth order (in \mathcal{E}) terms of (58 - 61):

$$e^{ik_j^0 L} = \prod_{\delta=1}^{M^u} \frac{\lambda_\gamma^0 - \sin k_j^0 - i\frac{u}{4}}{\lambda_\gamma^0 - \sin k_j^0 + i\frac{u}{4}} \prod_{l=1}^{N^b} \frac{\phi(q_l^0) - \sin k_j^0 - i\frac{u}{4}}{\phi(q_l^0) - \sin k_j^0 + i\frac{u}{4}} \quad (63)$$

$$\prod_{\delta \neq \gamma}^{M^u} \frac{\lambda_\gamma^0 - \lambda_\delta^0 - i\frac{u}{2}}{\lambda_\gamma^0 - \lambda_\delta^0 + i\frac{u}{2}} = \prod_{j=1}^{N^u} \frac{\lambda_\gamma^0 - \sin k_j^0 - i\frac{u}{4}}{\lambda_\gamma^0 - \sin k_j^0 + i\frac{u}{4}} \quad (64)$$

$$\prod_{\delta=1}^{M^u} \frac{\phi(q_l^0) - \lambda_\delta^0 - i\frac{u}{2}}{\phi(q_l^0) - \lambda_\delta^0 + i\frac{u}{2}} = \prod_{j=1}^{N^u} \frac{\phi(q_l^0) - \sin k_j^0 - i\frac{u}{4}}{\phi(q_l^0) - \sin k_j^0 + i\frac{u}{4}} e^{i\psi_l^0} \quad (65)$$

$$e^{2iq_l^0 L} = \prod_{\gamma=1}^{M^u} \frac{\lambda_\gamma^0 - \phi(q_l^0) - i\frac{u}{2}}{\lambda_\gamma^0 - \phi(q_l^0) + i\frac{u}{2}} \prod_{n \neq l}^{N^b} \frac{\phi(q_n^0) - \phi(q_l^0) - i\frac{u}{2}}{\phi(q_n^0) - \phi(q_l^0) + i\frac{u}{2}} e^{i\psi_l^0}. \quad (66)$$

The set (63 - 66) contains again the same number of unknowns as equations and should give the same solutions as (29,30,32) for the parameters $\{k_j^0\}, \{\lambda_\gamma^0\}, \{q_l^0\}$. In addition it determines the phases $e^{i\psi_l^0}$. Because we dropped only the exponentially small correction terms \mathcal{E} , the set $\{k_j^0, \lambda_\gamma^0, q_l^0, \Lambda_l^0 = \phi(q_l^0)\}$ deviates from $\{k_j, \lambda_\gamma, q_l, \Lambda_l\}$ only in quantities of order \mathcal{E} . Especially, if we choose an arbitrary l and define $\epsilon_l = e^{-\xi_l L}$, we can write

$$\begin{aligned} k_j(L) &= k_j^0(L) + k_j^{(1)}(L)\epsilon_l \\ \lambda_g(L) &= \lambda_g^0(L) + \lambda_g^{(1)}(L)\epsilon_l \\ q_l(L) &= q_l^0(L) + q_l^{(1)}(L)\epsilon_l \\ \Lambda_l(L) &= \phi(q_l^0(L)) + \Lambda_l^{(1)}(L)\epsilon_l \\ \chi_l(L) &= \frac{u}{4} + \chi_l^{(1)}(L)\epsilon_l. \end{aligned} \quad (67)$$

We will now show that the coefficient $\Lambda_l^{(1)}$ in (67) is determined through two independent equations, leading to an over-constraint.

One set of equations to determine $\Lambda_l^{(1)}$ is obtained as follows: dividing (3) for k_l^+ with (3) for k_l^- we get the following equation:

$$e^{-2\xi_l L} = \frac{(\Lambda_l - \phi(q_l))^2 + (\xi_l - \frac{u}{4})^2}{(\Lambda_l - \phi(q_l))^2 + (\xi_l + \frac{u}{4})^2} \prod_{\gamma}^{M^u} \frac{(\lambda_{\gamma} - \phi(q_l))^2 + (\xi_l - \frac{u}{4})^2}{(\lambda_{\gamma} - \phi(q_l))^2 + (\xi_l + \frac{u}{4})^2} \prod_{n \neq l}^{N^b} \frac{(\Lambda_n - \phi(q_l))^2 + (\xi_l - \frac{u}{4})^2}{(\Lambda_n - \phi(q_l))^2 + (\xi_l + \frac{u}{4})^2}. \quad (68)$$

which leads to,

$$1 = \frac{4}{u^2} \left(1 - \left[\frac{e^{i\psi_l^0} - 1}{e^{i\psi_l^0} + 1} \right]^2 \right) (\chi_l^{(1)})^2 f(\{\lambda_{\gamma}^0, q_n^0\}) \quad (69)$$

with f some function of $\{\lambda_{\gamma}^0, q_n^0\}$. This equation determines $\chi_l^{(1)}$ as function of the zeroth order variables $\{\lambda_{\gamma}^0, q_n^0, \psi_l^0\}$, therefore also the coefficient $\Lambda_l^{(1)}$ in (67), (using (62)), up to terms which are by themselves exponentially small. On the other hand, we obtain $\Lambda_l^{(1)}$ directly from eq. (60), by looking at the ϵ_l -correction. These two determinations of the coefficient $\Lambda_l^{(1)}$ are independent, as the former is derived from (3) and the latter from (4). This indicates that the set (58 - 61) is over-constrained in the first order finite volume correction to the thermodynamic limit. This effect can be studied in the three particle case by an explicit construction of the BA wave function assuming the $k - \Lambda$ string hypothesis. An over-determination of the parameters in expressions of order \mathcal{E} is found¹⁴. We conclude that the $k - \Lambda$ string hypothesis does not correspond to an actual solution of the BA equations for sufficiently large but finite L . The spectrum of the model on a finite ring is not in analytic one-to-one correspondence with the spectrum on the infinite line. On the other hand, the CBC - spectrum develops smoothly into the infinite volume limit, probably because it already contains an additional symmetry. This symmetry is presumably destroyed by the PBC and appears in this case only in the infinite volume limit.

Another way to observe the over-determination of (3,4) for finite volume is based on the algebraic Bethe ansatz.

We show that equations (60), which do not contain L explicitly, become redundant for $L \rightarrow \infty$, leading to superfluous constraints on the parameters: assume a pair of complex conjugated momenta k^+, k^- related to the spin momentum Λ by (7). An eigenstate of the corresponding inhomogeneous transfer matrix $Z(\mu)$ with (arbitrary) spectral parameter μ then has the form (see e.g. [5]): $|\psi\rangle = \prod_{\gamma=1}^{M^u} B(\lambda_{\gamma})B(\Lambda)|\omega\rangle$ for total spin $S = \frac{1}{2}(N^u - 2M^u)$, where the M^u creation operators $B(\lambda_{\gamma})$, acting on the ferromagnetic vacuum $|\omega\rangle$, create M^u \downarrow -spins, and $B(\Lambda)$ creates the \downarrow -spin of the bound state. By explicit calculation we find that $B(\Lambda)$ acting on $|\omega\rangle$ diverges as $e^{\frac{|u|}{4}L}$ for $L \rightarrow \infty$, whereas the B 's not associated with the complex pair do not diverge. Normalizing $|\psi\rangle$ by multiplication with $e^{-\frac{|u|}{4}L}$ yields accordingly an exponential suppression of vectors of the form $\prod_{\delta} B(\lambda_{\delta})|\omega\rangle$ which *do not* contain $B(\Lambda)$ among the $B(\lambda_{\delta})$. Now the equation (60) for Λ is necessary to cancel an “unwanted term” in the eigenvalue equation for $|\psi\rangle$:

$$(Z(\mu) - E(\mu))|\psi\rangle = \sum_{\gamma}^{M^u} \alpha_{\gamma} \prod_{\delta \neq \gamma}^{M^u} B(\lambda_{\delta})B(\Lambda)B(\mu)|\omega\rangle + \alpha_0 \prod_{\gamma}^{M^u} B(\lambda_{\gamma})B(\mu)|\omega\rangle. \quad (70)$$

It ensures, in particular, that $\alpha_0 = 0$. But, as argued previously, the vector $\prod_{\gamma} B(\lambda_{\gamma})B(\mu)|\omega\rangle$ is projected out in the infinite volume limit (exponentially suppressed for finite L), and therefore (60) is not necessary for $|\psi\rangle$ to be an eigenvector of $Z(\mu)$ for $L \rightarrow \infty$. That means that only a subset of all states allowed in the infinite volume can be generated by the $L \rightarrow \infty$ limit of string solutions to (3,4) for finite L .

In conclusion we find that the $k - \Lambda$ string hypothesis represents an over-constrained ansatz for solutions of BA equations for periodic boundary conditions, having in general no solutions for large but finite volume L .

III. GAPPED EXCITATIONS

In this section we will compute the simplest gapped excitations above the ground state for the repulsive and the attractive case. In the former case this amounts to the formation of a bound pair above the sea of unbound particles, in the latter case one of the bound pairs forming the ground state is broken and the resulting excitation has nonzero spin. Both excitations are characterized by a gap of order U and are accompanied, when the number of electrons is held fixed, by two gapless excitations: two holons in repulsive or two dressed electrons in the attractive case.

The range of the gapped excitation momentum, p^{bs} , depends on the filling n , $-\pi(1-n) \leq p^{bs} \leq \pi(1-n)$. At half filling it becomes therefore a non dynamic mode. We present the dispersion of the gapped mode for various fillings and interaction strengths.

A. The repulsive case

A single bound pair above the ground state of the repulsive Hubbard model can be created without changing the particle number N by placing two holes in the sea of the charge quantum numbers. $N^u = N - 2$ and $M = \frac{N}{2} - 1$ in the notation given above. Equations (29,30,32) then read²⁶,

$$Lk_j = 2\pi n_j + \sum_{\delta=1}^M \Theta_1(\sin k_j - \lambda_\delta) + \Theta_1(\sin k_j - \phi(q)) \quad (71)$$

$$\sum_{j=1}^{N-2} \Theta_1(\sin k_j - \lambda_\gamma) = \sum_{\delta=1}^M \Theta_2(\lambda_\delta - \lambda_\gamma) + 2\pi I_\gamma \quad (72)$$

$$2qL = \sum_{j=1}^{N-2} \Theta_1(\phi(q) - \sin k_j) + 2\pi J \quad (73)$$

where $\Theta_n(x) = \theta(x/n)$. The range for the quantum numbers $\{n_j\}$ is: $-N/2 \leq n_j \leq N/2 - 1$ for $M = N/2 - 1$ even and $-(N-1)/2 \leq n_j \leq (N-1)/2$ if M is odd. The $\{I_\gamma\}$ range between $-((N-2) - M - 1)/2$ and $+((N-2) - M - 1)/2$. The $\{n_j\}$ sequence contains two holes as the actual number of free k -momenta is $N - 2$. The $\{I_\gamma\}$ sequence does not contain holes in the absence of spin excitations. J , the quantum number associated with the bound state, is an integer if N is even and a half-odd integer if N is odd. We assume N even in the following. To find the limiting values for J , we consider the boundaries of the allowed range for q : $\pi/2 < q < \pi$, (resp. $-\pi < q < -\pi/2$). We may treat the range for q as connected by shifting $-\pi/2$ to $3\pi/2$. Setting $q = \pi/2$:

$$\pi L = 2\pi J^- - (N - 2)\pi \quad (74)$$

as $\phi(\pi/2) = \infty$. For $q = 3\pi/2$ we have $\phi(q) = -\infty$. Thus,

$$3\pi L = 2\pi J^+ + (N - 2)\pi. \quad (75)$$

Hence,

$$L - \frac{N}{2} > J > \frac{N}{2} \quad (76)$$

At half-filling: $(N/2) \leq J \leq (N/2)$, which leads to maximal restriction of the phase space for the bound state. In the infinite volume limit which is treated here, the phase space for J vanishes at half-filling. Recall that this is the case for spin singlet excitations where the string parameter is given in terms of the hole parameters⁵. The Lieb-Wu equations studied in [11] lead to a similar rigid relation between q , k_1 and k_2 , namely $\phi(q) = \frac{1}{2}(\sin k_1 + \sin k_2)$. While this rigidity holds at half-filling it is physically meaningless, as the physical momentum p^{bs} becomes *independent* of q at this point (see below).

We proceed now in the usual manner¹⁵, using the notation of [5]. One introduces the functions $\{\rho(k), \sigma(\lambda)\}$ to describe the densities of the $\{k\}$ and $\{\lambda\}$ solutions respectively. The ground state densities $\{\rho_0(k), \sigma_0(\lambda)\}$ are solutions of the appropriate integral equations with no holes in the distribution of the k_j , while the state under consideration now is given in terms of $\{\rho_b(k), \sigma_b(\lambda)\}$. The integral equations for these densities read,

$$\rho_b(k) + \frac{1}{L}\delta(k - k_1) + \frac{1}{L}\delta(k - k_2) =$$

$$\frac{1}{2\pi} + \cos k \int d\lambda \sigma_b(\lambda) K_1(\sin k - \lambda) + \frac{1}{L} \cos k K_1(\sin k - \phi(q)) \quad (77)$$

$$\sigma_b(\lambda) = \int_{-Q}^Q dk \rho_b(k) K_1(\sin k - \lambda) - \int d\lambda' \sigma_b(\lambda') K_2(\lambda - \lambda') \quad (78)$$

where k_1, k_2 denote the positions of the holes, and K_1, K_2 as well as R, \mathcal{K}^Q (see below) are kernels of integral operators defined as in [5]. The parameter Q defines the range of k and is given by,

$$\begin{aligned}\int_{-Q_0}^{Q_0} dk \rho_0^{Q_0} &= \frac{N}{L} \\ \int_{-Q}^Q dk \rho^Q &= \frac{N-2}{L}\end{aligned}\quad (79)$$

it depends therefore implicitly on k_1, k_2 and q . The equation for q reads,

$$2q = \frac{2\pi}{L}J + \int_{-Q}^Q dk \rho(k) \Theta_1(\phi(q) - \sin k). \quad (80)$$

It is convenient to introduce $\rho'_1(k), \sigma_1(\lambda)$,

$$\begin{aligned}\rho(k) &= \rho_0^Q(k) + \frac{1}{L}\rho'_1(k) - \delta(k - k_1) - \delta(k - k_2) \\ \sigma(\lambda) &= \sigma_0(\lambda) + \frac{1}{L}\sigma_1(\lambda)\end{aligned}\quad (81)$$

these correspond to the density changes induced by the excitations with respect to the density ρ_0^Q . The Fourier transform of the spin density $\sigma_1(\lambda)$ reads in terms of $\rho'_1(k)$,

$$\tilde{\sigma}_1(p) = \frac{1}{2} \int_Q^Q \rho'_1(k) \text{sech}\left(\frac{u}{4}p\right) e^{-ip \sin k} - \frac{1}{2} \text{sech}\left(\frac{u}{4}p\right) [e^{-ip \sin k_1} + e^{-ip \sin k_2}]. \quad (82)$$

It is possible to split $\rho'_1(k)$ into three parts

$$\rho'_1(k) = \rho_1^c(k, k_1) + \rho_2^c(k, k_2) + \rho^{bs}(k, q) \quad (83)$$

such that

$$\mathcal{K}^Q[\rho_j^c](k) = -\cos k \frac{4}{u} R \left(\frac{4}{u} (\sin k - \sin k_j) \right) \quad (84)$$

for $j = 1, 2$ and

$$\mathcal{K}^Q[\rho^{bs}](k) = \cos k K_1(\sin k - \phi(q)) \quad (85)$$

The excitation energy $\Delta E = E(Q) - E_0(Q_0)$ is defined via

$$\begin{aligned}E_0(Q) &= -2tL \int_{-Q}^Q dk \rho_0^Q(k) \cos k \\ E(Q) &= -2tL \int_{-Q}^Q dk \rho(k) \cos k\end{aligned}\quad (86)$$

With the usual definition of the chemical potential μ

$$\mu(Q) = \left(\frac{\partial E_0}{\partial N_0} \right) = \left(\frac{\partial E_0(Q)}{\partial Q} \right) \left(\frac{\partial N_0(Q)}{\partial Q} \right)^{-1} \quad (87)$$

and

$$N_0(Q) = L \int_{-Q}^Q dk \rho_0^Q \quad (88)$$

It follows

$$\Delta E = -2t \int_{-Q}^Q dk \rho'_1 \cos k + 2t[\cos k_1 + \cos k_2] - \mu(Q_0) \int_{-Q}^Q dk \rho'_1 \quad (89)$$

μ is independent of k_1, k_2 and q and given by Coll's formula¹⁵:

$$-\frac{\mu(Q_0)}{2t} = \frac{\cos(Q_0) - \int_{-Q_0}^{Q_0} dk \cos k \rho^c(k, Q_0)}{1 - \int_{-Q_0}^{Q_0} dk \rho^c(k, Q_0)} \quad (90)$$

The excitation energy is a sum of three parts

$$\Delta E = E_1^h + E_2^h + E^{bs} \quad (91)$$

Each of them consists of a direct, a backflow and a ground state contribution:

$$E_j^h(k_j) = 2t \cos k_j - 2t \int_{-Q}^Q dk \rho_c(k, k_j) \cos k - \mu \int_{-Q}^Q dk \rho_c(k, k_j) \quad (92)$$

The hole-energy goes to $-\mu$ for $k_j \rightarrow Q$. The bound state energy reads

$$E^{bs}(q) = -4t \cos q \cosh(\xi(q)) - 2t \int_{-Q}^Q dk \rho^{bs} \cos k - \mu \int_{-Q}^Q dk \rho^{bs}. \quad (93)$$

We proceed to discuss the energy dispersion. We shall do it for any filling. Consider the half filled case: using the identity $-4t \cos q \cosh(\xi(q)) = U + 2t \int_{-\pi}^{\pi} dk \cos^2 k K_1(\sin k - \phi(q))$ we see $E^{bs}(q) - U$ vanishes identically at half-filling and the dispersion of the excitation depends only on the hole part apart from the gap U .

Away from half-filling the bound state contribution becomes an independent excitation with its own dispersion. The momentum has contributions from the holes and from the bound state, given by,

$$\Delta P = P - P_0 = -p_1^h - p_2^h + p^{bs}. \quad (94)$$

The hole-momenta $\frac{2\pi}{L}n_j$ read

$$p_j^h = \int_0^{k_j} dk \rho_0(k) \quad (95)$$

(which leads to the identification of the point $k_j = \pm Q$ with the charge Fermi-momentum $\pm k_F = \pm \pi(N/L)$), while for p^{bs} we find

$$p^{bs}(q) = 2q - \int_{-Q}^Q dk \rho_0(k) \Theta_1(\phi(q) - \sin k). \quad (96)$$

As q runs over the allowed range $\pi/2 < q < \pi$ (resp. $-\pi < q < -\pi/2$), p^{bs} varies between $\pi + k_F$ and 2π (resp. $-2\pi < p^{bs} < -\pi - k_F$). This corresponds to a symmetric band around zero between $-|\pi - k_F|$ and $\pi - k_F$. It follows that at half-filling $p^{bs} \equiv 0$, i.e. the phase volume vanishes. The physical meaning of the shrinking to zero of parameter range at half filling has a simple interpretation: the bound state has no room to propagate. Although the bound state parameter q is fixed in this case, in terms of the hole parameters k_1 and k_2 ¹¹, this has no physical meaning: Energy and momentum, the physical parameters of the excitation, are *independent* of the unphysical parameter q , namely $E^{bs} \equiv U$ and $p^{bs} \equiv 0$. This redundancy of the parameter q at half-filling has led to some misconceptions in the literature²⁵.

Away from half-filling, the dispersion of the (always gapped) excitation is given parametrically by (93) and (96) for fixed hole-momenta k_1 and k_2 . We solved (84,85) numerically for $t = 1$ and two values of the interaction strength, $U = 0.5$ and $U = 2$. Figures 1 and 2 show the dispersion of the bound state energy $E^{bs}(p^{bs})$ for $U = 2$ and $U = 0.5$ respectively and for different values of the density n . Figures 3 and 4 show the dispersion curves for the same values of U , but for densities very close to half filling.

We notice that beyond a critical filling $n_c(U)$ the bound state energy dips below U . The critical value depends on U and decreases with increasing U . We are currently exploring whether the gap between the top of the holon and spinon bands and the bottom of the upper Hubbard band can actually close for some value of U .

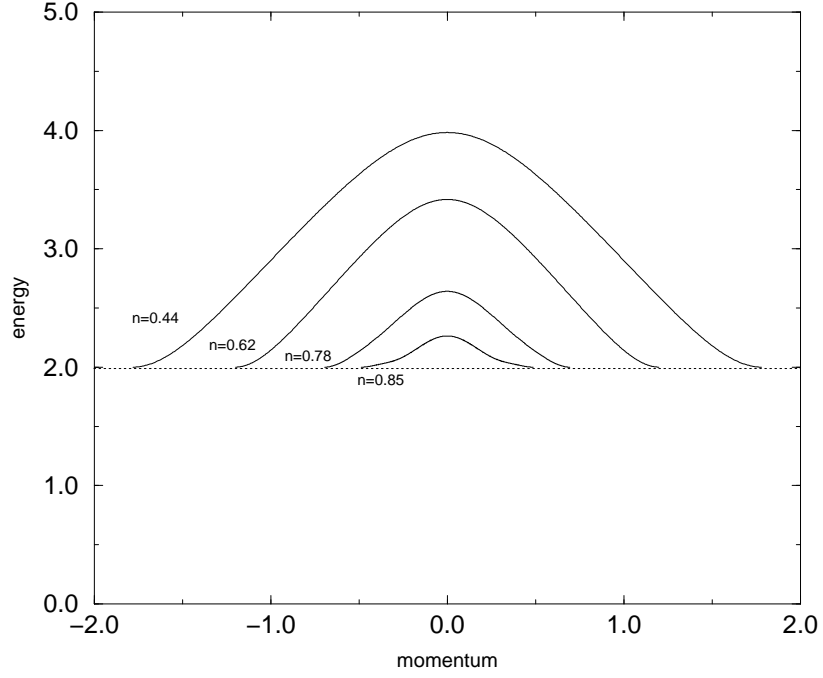


FIG. 1. The band of the bound state excitation for $U = 2$, and densities $n = 0.44, 0.62, 0.78$ and 0.85 , respectively.

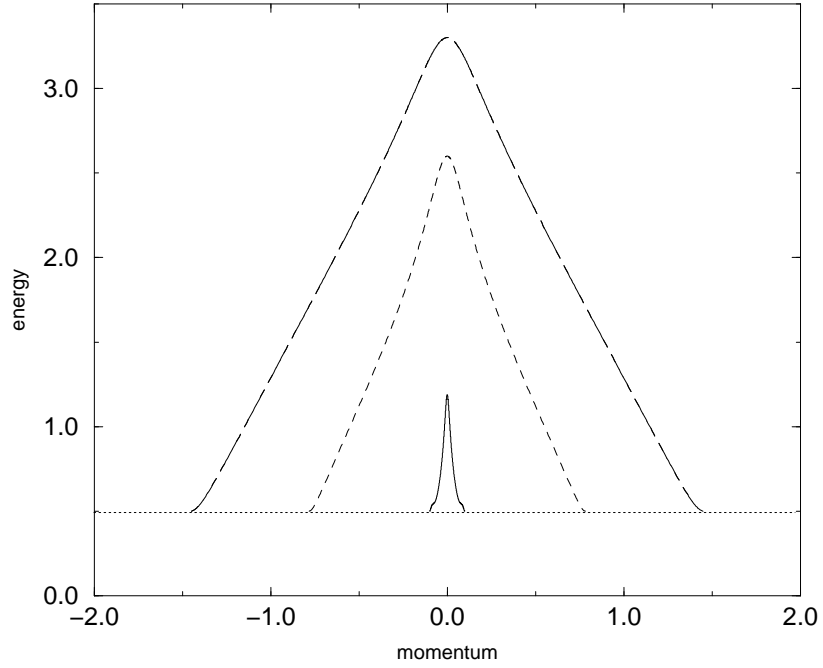


FIG. 2. The band for $U = 0.5$ and three values for the density, $n = 0.53$ (long-dashed), $n = 0.75$ (dashed), and $n = 0.96$ (solid line).

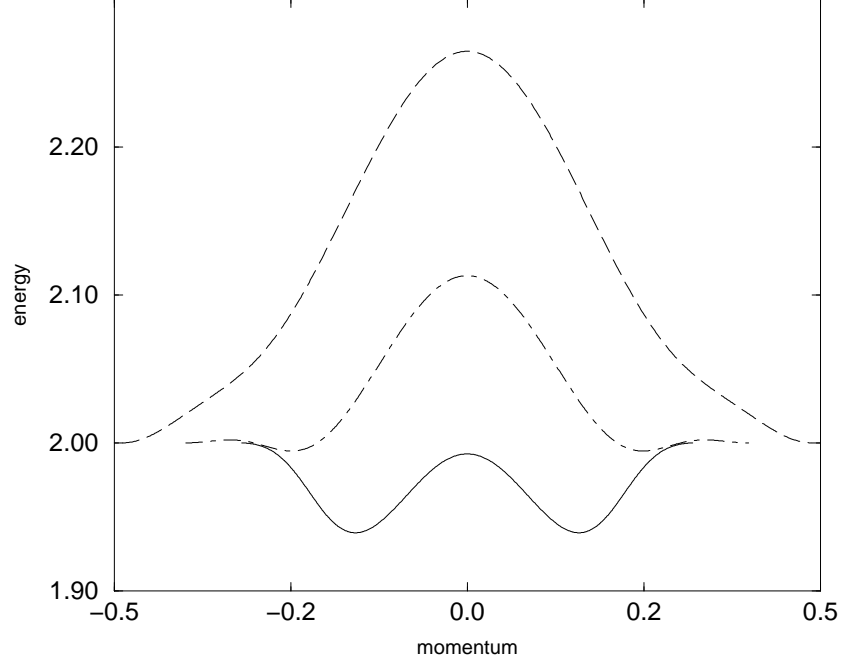


FIG. 3. The dispersion for $U = 2$ and $n = 0.84$ (long-dashed), $n = 0.87$ (dot-dashed) and $n = 0.89$ (solid line). The critical density $n_c \sim 0.86$.

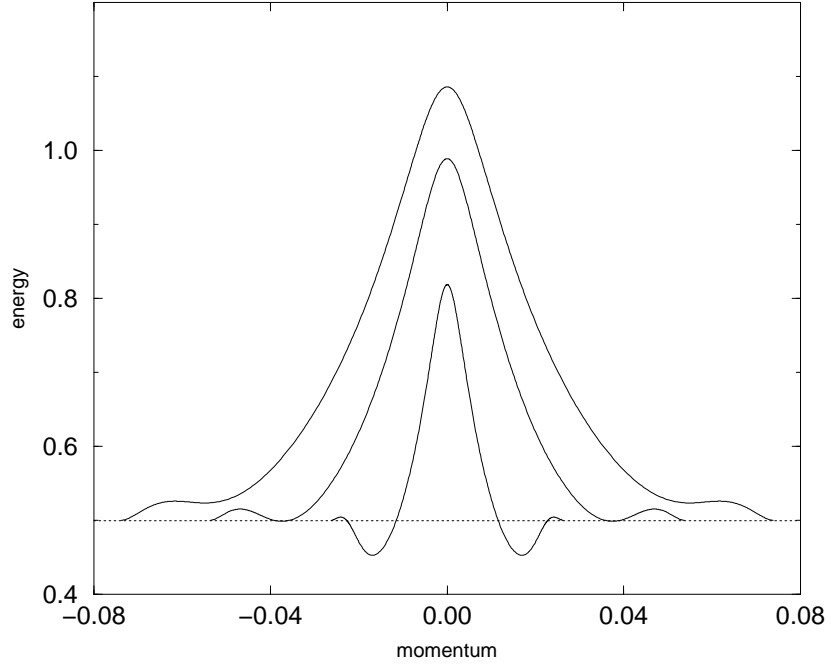


FIG. 4. The dispersion for $U = 0.5$ and three densities close to half filling: $n = 0.97, 0.98$ and 0.99 . The critical density $n_c = 0.98$.

B. The attractive case

In the attractive case $U < 0$ and we expect the ground state to consist solely of bound pairs (for even N), being a total spin singlet with $N^b = N/2$ and $N^u = M^u = 0$. We find accordingly,

$$e^{2iq_l} = \prod_{n \neq l}^{N^b} \frac{\phi(q_n) - \phi(q_l) - i\frac{u}{2}}{\phi(q_n) - \phi(q_l) + i\frac{u}{2}} \quad (97)$$

a reduced form of (32). We proceed in analogy with the treatment in section III A. The set of the q_l lies in the interval $-\frac{\pi}{2} < q_l < \frac{\pi}{2}$. Taking the logarithm of (97)

$$2q_l L = 2\pi J_l - \sum_{n \neq l}^{N^b} \Theta_2(\phi(q_l) - \phi(q_n)) \quad (98)$$

The range for the quantum number J_l , corresponding to the range for q_l above, is

$$-(L - N^b - 1)/2 < J_l < (L - N^b - 1)/2 \quad (99)$$

i.e. J_l is integer (half-odd-integer) if $L - N^b$ is odd (even). At half-filling $N = L$, the J_l 's are filling all the slots allowed by (99). It is convenient to change variables from q_l to $\phi(q_l)$, in defining the density, $L\sigma(\phi) = dJ/d\phi(q)$ which leads to the ground state integral equation,

$$\mathcal{L}^{B_0}[\sigma](\phi) = \frac{1}{\pi} F(\phi) \quad (100)$$

with $\mathcal{L}^{B_0}[\sigma](\phi) = \sigma(\phi) + \int_{-B_0}^{B_0} d\phi K_2(\phi - \phi')\sigma(\phi')$ and the inhomogeneous term, $F(\phi) = dq(\phi)/d\phi = \Re[1/\sqrt{1 - (\phi + i\frac{u}{4})^2}]$. As observed in [5], operator \mathcal{L}^B plays the same role as \mathcal{K}^Q in the repulsive case. The integration limit B_0 is determined by $\int_{-B_0}^{B_0} \sigma(\phi) d\phi = N^b/L$. At half-filling the r.h.s. is $1/2$, allowing us to deduce from that $B_0 = \infty$, and the equation can be solved via Fourier transformation⁵.

We now consider the simplest gapped excitations above this ground state. It involves pair-breaking, and is therefore a spin excitation.

We consider first the triplet: it is created by removing one bound pair and adding two free particles in a triplet spin state. We have,

$$2q_l L = 2\pi J_l - \sum_{n \neq l}^{N^b-1} \Theta_2(\phi_l - \Phi_n) - \Theta_1(\phi_l - \sin k_1) - \Theta_1(\phi_l - \sin k_2) \quad (101)$$

$$k_j L = 2\pi n_j - \sum_l^{N^b-1} \Theta_1(\sin k_j - \phi_l) \quad (102)$$

for $j = 1, 2$. The total spin is $S = 1$, $N^b \rightarrow N^b - 1$, $N^u = 2$, $M^u = 0$.

At half-filling the number of available slots is reduced by one (see (99)), therefore no hole opens in the J -sequence. The parameter of the excitation are just the two momenta of the free particles k_1 and k_2 . Away from half-filling $N = 2N^b < L$ and not all allowed slots are occupied in the ground state. Now, $B_0 < \infty$, the J_l 's are distributed symmetrically around zero and $|q_{max}| < \pi/2$. That means, we can create a hole in the J -sequence at position J_h , which corresponds to a $|\phi_h| < B_0$ although the number of allowed slots decreases by one. This J_h is the third parameter of the spin-triplet excitation and corresponds to the bound state parameter in the repulsive case. We proceed by introducing the densities, $\sigma(\phi) = \sigma_0^B(\phi) + \frac{1}{L}\sigma_1(\phi)$ and $\sigma_1(\phi) = \sigma_1'(\phi) - \delta(\phi - \phi_h)$ where $\sigma_0^B(\phi)$, being the ground state distribution with Fermi level B rather than B^0 , is determined by the normalization condition $\int_{-B}^B \sigma(\phi) d\phi = (N^b - 1)/L$.

Expressing the smooth density $\sigma_1'(\phi)$ as a sum of three terms, $\sigma_1'(\phi) = \sigma_c^1(\phi) + \sigma_c^2(\phi) + \sigma_h(\phi)$ we find,

$$\mathcal{L}^B[\sigma_c^j](\phi) = -K_1(\phi - \sin k_j) \quad (103)$$

for $j = 1, 2$ and

$$\mathcal{L}^B[\sigma_h(\phi, \phi_h)](\phi) = K_2(\phi - \phi_h). \quad (104)$$

Having solved (103,104) for the densities σ_c^j, σ_h , we compute the excitation energy. The total excitation energy consists of three terms,

$$\Delta E = E_1 + E_2 + E_h = -2t \sum_{j=1}^2 \cos k_j - \mathcal{E}(\phi_h) + \int_{-B_0}^{B_0} \mathcal{E}(\phi) \sigma_1'(\phi) - \mu^\sigma(B_0) \int_{B_0}^{B_0} \sigma_1'(\phi), \quad (105)$$

associated with the two unbound electrons and the *independent* hole respectively,

$$E_j = -2t \cos k_j + \int_{-B_0}^{B_0} \sigma_c^j(\phi) [\mathcal{E}(\phi) - \mu^\sigma] \quad (106)$$

$$E_h = -\mathcal{E}(\phi_h) + \int_{-B_0}^{B_0} \sigma_h(\phi, \phi_h) [\mathcal{E}(\phi) - \mu^\sigma]. \quad (107)$$

μ^σ is the chemical potential and accounts for the shift of the Fermi momentum $q(B)$ through the excitation. It is defined with respect to the number of bound pairs, $\mu^\sigma = dE_0/dN^b$, and given by an analog to (90):

$$\mu^\sigma(B_0) = \frac{\mathcal{E}(B_0) - \int_{-B_0}^{B_0} \mathcal{E}(\phi) \sigma_h(\phi, B_0)}{1 - \int_{-B_0}^{B_0} \sigma_h(\phi, B_0)}. \quad (108)$$

$\mathcal{E}(\phi)$ denotes the bound state energy function,

$$\mathcal{E}(\phi) = -4t \Re \sqrt{1 - (\phi + i \frac{u}{4})^2} \leq -|U|. \quad (109)$$

At half-filling $\sigma_h(\phi, \infty) \equiv 0$ and $\mu^\sigma(\infty) = -|U|$, as expected⁵.

The momenta p_j ; p_h , associated with the dressed electrons $j = 1, 2$ and the hole respectively, are given by,

$$p_h = \int_0^{\phi_h} \sigma_0^{B_0}(\phi) \quad (110)$$

$$p_j = k_j + \int_{-B_0}^{B_0} d\phi \Theta_1(\sin k_j - \phi). \quad (111)$$

Removing the bound state at the Fermi level B we have,

$$p_h(B) = \pi \frac{N^b}{L} = \frac{\pi}{2} n \quad (112)$$

which identifies the Fermi momentum in the attractive case, $k_F^{att} = \frac{\pi}{2} n$. Note also that the dressed momenta p_j of the two unbound electrons deviate from their free values k_j . The hole contribution to energy and momentum, given by E_h and p_h in (107) and (110), play the same role as E^{bs} and p^{bs} in section III A.

Now consider the singlet excitation. We break a pair and put the two electrons into a spin singlet state. Again N^b is reduced by one, leading to an additional degree of freedom away from half-filling. $N^u = 2$, but $M^u = 1$ and $S = 0$, the total spin is not changed. We have one λ parameter for the unbound electrons. Equation (30) reads then,

$$1 = \frac{\lambda - \sin k_1 + i \frac{|u|}{4}}{\lambda - \sin k_1 - i \frac{|u|}{4}} \frac{\lambda - \sin k_2 + i \frac{|u|}{4}}{\lambda - \sin k_2 - i \frac{|u|}{4}} \quad (113)$$

which leads to the familiar form

$$\lambda = \frac{1}{2} (\sin k_1 + \sin k_2). \quad (114)$$

Eq. (101) remains valid in the singlet case while eq. (102) becomes

$$k_j L = 2\pi n_j - \sum_l^{N^b-1} \Theta_1(\sin k_j - \phi_l) - \Theta_1(\sin k_j - \lambda) \quad (115)$$

The effect of this modification is to change the relative phase shift of the particles,

$$\delta^{singlet} = \delta^{triplet} - \Theta_2(\sin k_1 - \sin k_2) \quad (116)$$

as expected on general grounds⁵.

We have analyzed the simplest gapped excitations. In the repulsive case, when the number of electrons is held fixed, the spectrum consists of two gapless holons, as well as a gapful singlet residing in the upper Hubbard band. We have calculated its dispersion for various values of the filling and interaction strength, see figure (1,2,3). The gapped excitations are independent of the concomitant holon excitations away from half-filling. A dual picture holds for the attractive case.

The upper Hubbard excitation we discussed was based on a two-particle bound state; other excitations emerge when higher composites are studied, and can be identified with elementary m -complexes, see eq.(37). These have higher gaps with respect to the ground state and constitute the upper bands.

IV. SUMMARY

We have studied in this article the gapful excitations of the one-dimensional Hubbard model, constituting the upper Hubbard band. We have introduced a simple and intuitive construction to incorporate complex momenta solutions that correspond to these states. Our analysis has the following results:

- 1) In infinite volume states with complex momenta are (elementary) bound states of the hamiltonian, formed of any (even) number of electrons. These states are spin singlets and live in the upper Hubbard band for $U > 0$ and the lower band for $U < 0$. They are renormalized by interacting with other particles, bound or unbound.
- 2) These states exist for finite volume if Composite Boundary Conditions (CBC) are introduced. Their existence can be proven exactly without postulating a string-hypothesis, via the Bethe Ansatz for Composites (BAC) approach. We have shown that all states can be obtained within this scheme.
- 3) We clarified the physical interpretation of the $SU(2)_{charge}$ symmetry in the framework of BAC and have shown that it corresponds to the addition of completely local bound states. A simple proof for the corresponding lowest weight property of the Bethe states follows.
- 4) We have argued that the states with complex momenta *cannot* have the string form for large but finite volume and periodic boundary conditions (PBC). That means that the $k - \Lambda$ string hypothesis may give correct results in the thermodynamic limit but fails for finite volume and PBC.
- 5) The simplest gapped elementary excitations involve a multi-particle bound state. When the number of electrons is held fixed the presence of such a state is accompanied by the appearance of at least two holons in the repulsive case or two dressed electrons in the attractive case. The gapped excitation is an independent mode only away from half filling, becoming a non-dispersive gap at half filling.

We conclude with two conjectures. The first is related to the possibility of the BAC construction, which follows from the composite boundary conditions: we conjecture that the CBC incorporate a symmetry algebra which should be similar to the Yangian symmetry found up to now only in infinite systems.

Furthermore, we conjecture that for a finite system with periodic boundary conditions the Hubbard model is no longer integrable in the strong sense; that means the wavefunctions in the N -particle sector with spin S cannot be parameterized by the set $\{k_j, \lambda_j\}$ of N momenta and $N/2 - S$ spin rapidities alone, if some of the momenta are complex.

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A. Appendix - Derivation of eq.(25)

This appendix contains the detailed derivation of (25), thereby showing the stability of the two-particle bound state if it satisfies the pole condition (10). We define $S_{1(23)}^{ub}$ by,

$$A_{[231]}^{a_1 a_2 a_3} = S_{1(23)}^{ub}(k, q^-, q^+) A_{[123]}^{a'_1 a'_2 a'_3} \quad (117)$$

i.e. it takes particle 1 with the real momentum k from the left side of the bound pair to the right side, without changing their momenta. In both the initial and final amplitudes, we have particle 2 on the left of particle 3, which means $k_2 = q^-$ and $k_3 = q^+$. Therefore, $S_{1(23)}^{ub}$ is given as the product,

$$S_{1(23)}^{ub}(k, q^-, q^+) = S_{13}^{uu}(k, q^+) S_{12}^{uu}(k, q^-) \quad (118)$$

which is equation (24). To proceed we write $S^{uu}(k_a, k_b)$ in the form

$$S_{ab}^{uu}(k_a, k_b) = \frac{1}{2}(1 + s_{ab})\mathbf{1} + \frac{1}{2}(1 - s_{ab})P_{ab} \quad (119)$$

where P_{ab} is the spin exchange operator between particles a and b . The phase s_{ab} depends on k_a and k_b as,

$$s_{ab} = \frac{\sin k_a - \sin k_b - i\frac{u}{2}}{\sin k_a - \sin k_b + i\frac{u}{2}}. \quad (120)$$

We write

$$s_- = \frac{\sin k - \sin q_- - i\frac{u}{2}}{\sin k - \sin q_- + i\frac{u}{2}} \quad s_+ = \frac{\sin k - \sin q_+ - i\frac{u}{2}}{\sin k - \sin q_+ + i\frac{u}{2}}. \quad (121)$$

Then

$$\begin{aligned} S_{1(23)}^{ub} &= \left(\frac{1}{2}(1 + s_+) + \frac{1}{2}(1 - s_+)P_{13} \right) \left(\frac{1}{2}(1 + s_-) + \frac{1}{2}(1 - s_-)P_{12} \right) \\ &= \frac{1}{4} [(1 + s_+)(1 + s_-) + (1 + s_-)(1 + s_+)P_{13} \\ &\quad + (1 + s_+)(1 + s_-)P_{12} + (1 - s_+)(1 - s_-)P_{13}P_{12}]. \end{aligned} \quad (122)$$

Now we use the fact that the spin space of the three particles is restricted: 2 and 3 are in a mutual singlet in region [123]. The spin state space in this region is therefore $V_A = V_1 \otimes V_{23}^{singlet}$ and a two-dimensional subspace of the eight-dimensional spin space of the three particles. Under this condition $P_{23}A_{[123]} = -A_{[123]}$. It follows then $P_{13}P_{12} = P_{12}P_{23} = -P_{12}$ if acting on V_A . A further identity valid if the operators act on V_A reads $P_{12} = \mathbf{1} - P_{13}$. Note that these operators do not leave V_A invariant. In general, therefore, the singlet state of particles 2 and 3 will be destroyed upon scattering with particle 1. It is due to a non trivial cancelation of terms if momenta q^+ , q^- satisfy the pole condition for S_{23}^{uu} , that $S_{1(23)}^{ub}$ indeed leaves V_A invariant and acts as a pure spin independent phase on the wavefunction. We use the identities above to simplify expression (122) and find

$$S_{1(23)}^{ub} = \frac{1}{4} [(1 + s_-)(1 + s_+) + 2s_+(1 - s_-)] + P_{13}[1 + s_- - 3s_+ + s_+s_-]. \quad (123)$$

Explicit calculation shows that the term multiplying P_{13} vanishes for q^+, q^- satisfying the pole condition (10). It follows that $S_{1(23)}^{ub}$ is indeed proportional to the identity on V_A , leaving the bound state invariant up to a phase:

$$S_{1(23)}^{ub} = \frac{1}{2}(1 + s_-) = \frac{\sin k - \phi(q) - i\frac{u}{4}}{\sin k - \phi(q) + i\frac{u}{4}} \quad (124)$$

In an analogous manner one writes for the S-matrix of two bound states, consisting of particles 1 and 2 parameterized by $\phi(q_{12})$ and 3 and 4, parameterized by $\phi(q_{34})$,

$$S_{(12)(34)}^{bb} = S_{1(34)}^{ub} S_{2(34)}^{ub} \quad (125)$$

and one finds immediately

$$S_{(12)(34)}^{bb} = \frac{\phi_{12} - \phi_{34} - i\frac{u}{2}}{\phi_{12} - \phi_{34} + i\frac{u}{2}}. \quad (126)$$

- ¹ F. H. L. Essler, V. E. Korepin and K. Schoutens, Nucl.Phys **B372**, (1992) 559.
- ² D. Braak and N. Andrei, preprint Rutgers University, RU-98-23, cond-mat/9805103.
- ³ M. Takahashi, Prog. Theor. Phys. **47**, (1972) 69.
- ⁴ E. L. Lieb and F. Y. Wu, Phys. Rev. Lett **20**, (1968) 1445.
- ⁵ For a detailed derivation see: N. Andrei, in *Series on Modern Condensed Matter Physics*, Vol. 6, Summer Course (1992), Lecture Notes of the ICTP, 458 - 551; cond-mat/9408101.
- ⁶ See however, N. Andrei, D. Braak and A. Deppeler, Rutgers preprint (in preparation).
- ⁷ N. Andrei and J. H. Lowenstein, Phys. Rev. Lett. **43**, (1979) 1698.
- ⁸ N. Andrei and J. H. Lowenstein, Phys. Lett. **91B**, (1980) 401.
- ⁹ N. Andrei, Phys. Rev. Lett. **45**, (1980) 379.
- ¹⁰ L. D. Faddeev and L. A. Takhtajan, Physics Lett. **85A**, (1981) 375.
- ¹¹ F. Woynarovich, J. Phys **C15** (1982) 85; ibid. 97; ibid. **C16**, (1983) 5293.
- ¹² P. A. Bares, G. Blatter and M. Ogata, Phys. Rev **B 44**, (1991) 130.
- ¹³ C. N. Yang, Phys. Rev. **168**, (1968) 1920.
- ¹⁴ D. Braak, Notes '98.
- ¹⁵ C. F. Coll, Phys. Rev. **B 9**, (1974) 2150.
- ¹⁶ C. N. Yang, Phys. Rev. Lett. **63**, (1989) 2144.
- ¹⁷ I. Affleck, in *Banff Lectures*, Nato Advanced Study in Physics (1989).
- ¹⁸ F. H. L. Essler, V. E. Korepin and K. Schoutens, Nucl. Phys. **B384**, (1992) 431.
- ¹⁹ We thank P. Zinn-Justin for illuminating discussions on the subject.
- ²⁰ The argument actually requires sharpening: a Z_2 symmetry needs to be respected.
- ²¹ It is interesting to note the simplicity of the proof as compared with the one in Ref.[1], which extends on 15 pages. Their main theorem (2.1), stating that $\eta^+|0\rangle$ is not a BA state, is wrong since the possibility of complex momenta is not considered.
- ²² Equations (58,59,61,60) are algebraically independent. They also have as a consequence the quantization condition of the total momentum on a ring,

$$e^{i(\sum_j k_j + 2 \sum_l q_l)L} = 1.$$

The latter is derived as follows. Take the product of equations (58) over all j with the product of equations (61) over all l :

$$e^{i(\sum_j k_j + 2 \sum_l q_l)L} = \prod_j^{N^u} \prod_l^{N^b} \prod_{\delta=1}^{M^u} \frac{\lambda_\gamma - \sin k_j - i\frac{u}{4} \Lambda_l - \sin k_j - i\frac{u}{4} \lambda_\gamma - \Lambda_l - i\frac{u}{2}}{\lambda_\gamma - \sin k_j + i\frac{u}{4} \Lambda_l - \sin k_j + i\frac{u}{4} \lambda_\gamma - \Lambda_l + i\frac{u}{2}} e^{i\psi_l}.$$

Using now eq.(59) and the trivial identity, $\prod_{\delta, \gamma, \delta \neq \gamma}^{M^u} \frac{\lambda_\gamma - \lambda_\delta - i\frac{u}{2}}{\lambda_\gamma - \lambda_\delta + i\frac{u}{2}} = 1$, it follows,

$$e^{i(\sum_j k_j + 2 \sum_l q_l)L} = \prod_l^{N^b} \prod_\gamma^{M^u} \frac{\lambda_\gamma - \Lambda_l - i\frac{u}{2}}{\lambda_\gamma - \Lambda_l + i\frac{u}{2}} \prod_{j=1}^{N^u} \frac{\Lambda_l - \sin k_j - i\frac{u}{4}}{\Lambda_l - \sin k_j + i\frac{u}{4}} e^{i\psi}. \quad (127)$$

Equations (60), which set the right hand side of eqn (127) equal to 1, have as a consequence, as asserted, that the total momentum is quantized.

It was attempted by Essler et al.²³ to show that eq.(60) follows algebraically from the set (58,59,61). They restricted their attention to the simpler case of a single bound state and set $e^{i(\sum_j k_j + 2q)L} = 1$, this way they simply assumed what was to be proven²⁴.

²³ F.H.L. Essler, F. Goehmann and V.E. Korepin, cond-mat/9806125.

²⁴ D. Braak and N. Andrei, cond-mat/9806225.

²⁵ Reference [23] provides an example of such misconceptions.

²⁶ F. D. M. Haldane and Y. Tu, UCSD preprint (1989).